SOLVING LARGE-SCALE DYNAMIC SYSTEMS USING BAND LANCZOS METHOD IN ROCKWELL NASTRAN ON CRAY X-MP

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SUMMARY

The improved cost-effectiveness using better models, more accurate and faster algorithms, and large-scale computing offers more representative dynamic analyses. The band Lanczos eigen-solution method has been implemented in Rockwell's version of 1984 COSMIC-released NASTRAN finite-element structural analysis computer program to effectively solve for structural vibration modes including those of large complex systems exceeding 10,000 degrees of freedom.

The Lanczos vectors are re-orthogonalized locally using the Lanczos Method and globally using the modified Gram-Schmidt method for sweeping rigid-body modes and previously generated modes and Lanczos vectors. The truncated band matrix is solved for vibration frequencies and mode shapes using Givens rotations. Numerical examples are included to demonstrate the cost-effectiveness and accuracy of the method as implemented in ROCKWELL NASTRAN. The CRAY version is based on RPK's COSMIC/NASTRAN.

The band Lanczos method is more reliable and accurate and converges faster than the single vector Lanczos Method. The band Lanczos method is comparable to the subspace iteration method which is a block version of the inverse power method. However, the subspace matrix tends to be fully populated in the case of subspace iteration and not as sparse as a band matrix.

INTRODUCTION

With the objective of solving large-scale dynamic systems, several papers in recent years have presented a number of issues, of which we address, in particular, the following.

The improved cost-effectiveness with large-scale computing offers more extensive optimization (1-4), nonlinear capability (5), and more representative dynamic analyses(3-7), in addition to solution of fluid mechanics problems.

A cheaper solution to the larger numerical problem does not, however, eliminate the desire for solving the problems of proper formulation, modelling, and interpretation of results, using expert systems, in an effort to capture the finite-element modelling expertise of real-world aircraft structures, which involves decisions about mesh size, element selection, and constraint representation. Compatible system development is, however, the key to integrating software "black boxes" associated with the finite element analysis that generates most of the data, the data base management systems that handle and store the data, and the user-friendly interfaces that display the data; this, ideally, should be achieved by design rather than by adaptation. Grooms, Merriman, and Hinz (8) are developing an expert system for training structural engineers in modelling and analyses using ROCKWELL NASTRAN.

The correlation between a real physical structure and its mathematical finite element model (FEM) is premised on reasonable and defensible assumptions and idealizations. The agreement between experiment and theoretically predicted frequencies becomes weaker for the higher modes. With enough modelling elements, the FEM model for a complicated structure can, in principle, be made arbitrarily accurate. To achieve modal convergence, Hughes (9) computes modal coefficients of both momentum and angular momentum to identify dominant modes that must be retained when the number of Lanczos vectors is truncated . He analyzes a wrap-rib space antenna reflector by re-ordering modes, selecting only 9 dominant ones instead of the 26 suggested by the simple natural order modal truncation procedure based on experience with slender beam models. He found breathing modes to be important for the sake of convergence. Hughes' mode selection criteria tends to reduce the cost of dynamic response based on modal superposition.

The problem size or dimensionality can be reduced by Guyan reduction (10,11), e.g., at substructure level (5), and

component mode synthesis (12,13), by omitting unnecessary elastic degrees of freedom to suppress insignificant modes. For a large sparse system, dynamic condensation and associated loss of sparsity tends to increase eigensolution cost (14); the Lanczos method offers a superior alternative, since it does not rely on adhoc degree-of-freedom selection without apriori knowledge of modes to achieve reduced problem size. For a linear structural dynamic system, which is inertia invariant when the gross body motion is small, the frequency spectrum of the system transfer function is independent of time. A number of dominant modes of vibration can be retained, e.g., based on Fourier analysis of the frequency spectrum of the forcing function. The load-dependent basis of Ritz vectors, which are equivalent to Lanczos vectors, can be exploited to minimize the cost of dynamic analysis, linear (7,15,16) or nonlinear (17). However, the frequency content of the external forcing functions alone is not sufficient for predicting excitation of closely spaced modes in the system, if mass matrix changes or nonlinear effects cause inertia-induced reaction forces to excite higher modes. With damping, higher modes need to be retained only over short transients, not over the entire time interval. The static effect of higher modes can be accounted for by either including certain correction terms with modal superposition, as suggested by Shabana and Wehage (13), and Misel et al (6), or by peforming dynamic analysis in terms of Ritz or Lanczos vectors (7,15-17).

Local buckling of a conventional aircraft wing, preferrably based on a sufficiently detailed representation of the reinforcing stiffeners and any substantial features (e.g., access holes, mounting lugs, etc.), could result in a mesh of approximately 100,000 nodes - one order of magnitude beyond current practice. With multi-level substructuring, analyses of up to 500,000 degrees of freedom have been performed. The development of automated modelling and advanced hardware-software systems in the next ten years may lead to bigger analysis involving one to ten million degrees of freedom.

BAND LANCZOS METHOD

The band Lanczos method (18,19) is similar to the one called block Lanczos (20-22), or Subspace Iteration (15,16,23,24), or block Stodola (25), or Simultaneous Iteration (24), all involving simultaneous iteration using a block of trial vectors; their authors - Hestenes and Karush,

Bauer, Rutishauser, Jennings and Orr, Dong, Wolf, and Peterson, Bathe and Wilson - are referenced by Parlett (19), Bathe (24), or Dong (25). In contrast, classical Stodola-Vianello technique (also known as inverse power method) and simple Lanczos method (14,26-28) operate on one trial vector rather than a block of vectors. The band or block approach has been demonstrated to be effective and very efficient computationally when solving sparse algebraic system with large bandwidth for subset of the lowest eigenvalues and corresponding eigenvectors. Dong (25) has further extended the Block Stodola method to solve the complex, quadratic, and cubic eigenvalue problems.

Assume an algebraic eigensystem of the form: Ku = e Mu, where K and M cannot both be singular but both are symmetric and large and preferably narrowly banded, i.e., not involving damping, Coriolis effects and non-conservative forces which make K unsymmetric. The Lanczos method essentially reduces the rank of the algebraic eigensystem by an appropriate transformation. The starting vectors selected must span the dominant subspace eigenbasis in a relatively complete mathematical sense by not being orthogonal to this subspace. If the transformation T spans the dominant subspace completely, the eigenvectors are true and the solution is exact. The subset of eigenvectors in the original space is recovered by T. The band Lanczos method when applied to structural problems is similar to Ritz analysis in that eigenvalues are upper bounds and convergence will always be from above; the extent to which this frequency discrepancy is affected by Guyan reduction depends upon the degrees of freedom selected. Though not necessary in the case of band Lanczos method, Sturm sequence technique(29) has been suggested to ensure and verify convergence of all of the dominant eigenvalues with the subspace iteration technique, along with some shifting strategy (23). Frequency shifting accelerates convergence of modes near the shift frequency. Wilkinson (30) analogizes Lanczos method to the Stodola power iteration with shifts.

Shifted Block Lanczos Method has been implemented in MSC/NASTRAN (21,22) for Version 65. A procedure re-orthognalizes Lanczos vectors to maintain accuracy, while multiple frequency shifts permit spanning higher modes in the eigenspectrum. The decision to shift involves a trade-off between convergence error and the cost of triangular decomposition required at each frequency shift. Other performance tradeoffs by Grimes et al (22) show that the input/output cost will vary inversely as the block size, and the CPU cost will vary directly. Parlett (32) also recommends

the block approach with larger block size for problems that require more than available primary computer storage, as the input/output cost of reading and writing large matrices dominates the CPU cost.

Band Lanczos Algorithm

In an earlier paper(14), we described our implementation of the Lanczos-Householder algorithm in ROCKWELL NASTRAN (Level 17.5), based on simple Lanczos method (19,26,28) and Householder re-orthogonalization (31) with respect to all previously generated modes and Lanczos vectors. Weingarten (27) showed by three examples that this method "requires less CPU time than the standard subspace iteration and determinant search" techniques in SAP7. Parlett (32) compared explicitly vectorized versions of the simple Lanczos method and subspace iteration method on Cyber 205 and found the Lanczos method to be at least 10 times more CPU efficent. Several authors have demonstrated the block approach to be even more effective and efficient computationally when solving sparse algebraic eigensystems with large bandwidth for subset of the lowest eigenvalues and corresponding eigenvectors. We selected Parlett's (19) version of the band Lanczos method to enhance performance of the simple Lanczos algorithm in ROCKWELL NASTRAN on IBM and CRAY X-MP computers. However, a few modifications were made to improve the accuracy and cost-effectiveness of the algorithm in ROCKWELL's production version of the April 1984 COSMIC-released NASTRAN.

The modifications incorporated (14,26) are primarily concerned with the selection of starting trial vectors and block size, Householder/Gram-Schmidt re-orthogonalization (31,33,34), explicit/implicit vectorization on CRAY computer, dynamic core allocation, automatic restart with a new randomly generated vector when the Lanczos feed vector becomes null or dominated by numerical noise, and the truncation criteria to achieve the required number of converged eigenpairs.

Described as the FEER method in NASTRAN programmer's manual (28), the simple Lanczos method has been available in COSMIC-released NASTRAN since level 17.5 (1979), including Cholesky decomposition of the mass-shifted stiffnes matrix, forward-backward substitution, and recovery of the physical eigenvectors using Lanczos vectors to transform the truncated eigenvectors of the reduced eigenproblem. Cholesky decomposition is premised on a semi-positive definite matrix. The shift frequency is internally calculated, which permits

calculation of zero-order modes without making the resulting shifted matrix indefinite. Whether eigenvectors are ortho- or mass-normalized, the truncated band matrix is identical. The mathematical equations are well documented (14,26,28).

The band Lanczos method, as implemented in ROCKWELL NASTRAN, is useful for calculating modal frequencies near zero, particularly the fundamental frequencies and the lowest dominant modes. A built-in restart capability (14) assures convergence to maximum cut-off frequecy without a shift. For still higher-order interior modes, a frequency shift, if required, is possible using the simple Lanczos method or even the Inverse Power Method, by appending and sweeping out the modes previously calculated by the band Lanczos method.

Numerical Results

A series of numerical examples have been executed on ROCKWELL NASTRAN using IBM and CRAY versions to validate the Band Lanczos method for production use. Cray wall clock and CPU times are fraction of those for IBM. Rockwell's CRAY X-MP/14 (COS) has 4 million words of central memory to allow cost-effective solution of reasonably large dynamic problems.

The Band Lanczos method implementation affected NASTRAN READ Module subroutines FNXTVC, VALVEC, REIG, FEERBD, QRITER, and WILVEC, resulting in cost savings of 16% to 46% during READ Module execution over the FEER method, for different size problems. The COSMIC NASTRAN method FEER frequently fails to converge on a multiple root and the associated eigenvector. The reduced problem size necessary to determine q eigenpairs accurately was specified as (2q+10) for the FEER (simple Lanczos) method as well as the Band Lanczos method to assure convergence of q user-specified number of roots.

When Guyan reduction was used to reduce 2380 degrees of freedom to 494, the eigensolution time (READ module execution after triangular decomposition) to obtain 40 modes using the band Lanczos method was reduced from 203 CPU seconds to 176, whereas the overall solution time including the cost of Guyan condensation increased from 211 to 550. A comparison of eigensolution times for FEER (simple Lanczos method) and band Lanczos method as implemented in Rockwell's enhanced version of RPK's April 1984 release of Cray COSMIC/NASTRAN is also presented in Table 1. Rockwell's Cray NASTRAN has been partly optimized to take advantage of the available central memory, dynamically.

CONCLUDING REMARKS

Following are some distinct advantages of using the band Lanczos algorithm as implemented in ROCKWELL NASTRAN:

1. multiple or closely clustered roots can be accurately determined without the risk of missing them or without the necessity of a Sturm sequence property check; this risk seemingly exists with the simple or single-vector Lanczos method as well as the subspace iteration method.

2. local Lanczos re-orthogonalization in Parlett's Band Lanczos algorithm assures purity of the resulting Band matrix (19).

The use of Lanczos vectors looks promising for performing linear and nonlinear dynamic analyses, involving substructuring, in the spirit of component mode synthesis.

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TABLE 1 Time Comparison (CPU seconds)

Problem 1: 2380 Degrees of freedom, 2-D plate model			
Method:	Cosmic FEER	Rockwell Band LANCZOS	
Guyan Reduction:	NO	NO	YES
IBM 3081	307	203(211)	176(550)
IBM 3090	144	95(99)	79(216)
CRAY X-MP	90	48(52)	74(154)
Problem 2: 6006 Degrees of freedom, 8-node brick model			
CRAY X-MP	680	596(971)	--